

Numerical Modeling of Small Scale Water Mitigation Feasibility Tests

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This work was sponsored by the Naval Facilities Engineering Service Center, Port Hueneme, California under Contract No: N47408-97-M-0928

Report Documentation Page				Form Approved OMB No. 0704-0188	
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1. REPORT DATE AUG 1998		2. REPORT TYPE		3. DATES COVERED 00-00-1998 to 00-00-1998	
4. TITLE AND SUBTITLE Numerical Modeling of Small Scale Water Mitigation Feasibility Tests				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Century Dynamics, Incorporated, 2333 San Ramon Valley Blvd Suite 185, San Ramon, CA, 94583				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES See also ADM001002. Proceedings of the Twenty-Eighth DoD Explosives Safety Seminar Held in Orlando, FL on 18-20 August 1998.					
14. ABSTRACT see report					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 25	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

Abstract

Water placed in the vicinity of explosives in a confined environment has been found to significantly mitigate the quasi-static gas pressure from an explosion. Reports on several small scale tests available from the open literature confirm that gas pressures can be reduced by up to 90%. This is of significant importance for the safety of explosive facilities wherein the gas pressure from an explosion controls debris distance. Analytical and numerical models are needed to model the effects of water mitigation and to predict the resulting gas pressure.

A series of calculations using the AUTODYN software program were performed to simulate three small scale feasibility experimental tests of explosions inside rigid chambers. Each of the tests is represented in a simplified form by an axisymmetric two-dimensional model with and without the presence of water. Each test includes a configuration wherein the water is placed close to the explosive such that the explosive may be considered to be immersed in the water. In addition, in one of the test series, the water was placed only on the sides of the explosive in order to determine the effect of water placement on the final gas pressure.

The three simplified models were analyzed using AUTODYN in its standard release form. Additional calculations were then made with AUTODYN modified through use of a user subroutine to account for heat transfer effects not represented in the standard version of the program.

The correlation of numerical and experimental results for the bare charge situations was quite good. Introduction of the water into the tests, and using AUTODYN in its standard form, does provide a mitigation of the gas pressure, but not to the extent as evidenced in the experiments. When the effects of heat transfer between explosive products and water/vapor are included in the model, the gas pressures are further reduced to levels generally within the range observed in the experiments.

Such numerical modeling holds great promise for being able to study the water mitigation problem, not only in the simplified geometries studied herein, but in more complex situations as well.

1. Introduction

Water placed in the vicinity of explosives in a confined environment significantly mitigates the quasi-static gas pressure from an explosion. Reports on several small scale tests available from the open literature confirm that gas pressures can be reduced by up to 90%. This is of significant importance for explosive safety facilities where the gas pressure controls debris throw distance. This paper presents work in numerical modeling of the water mitigation process with emphasis on validation of numerical results with experiment.

A series of calculations using the AUTODYN software program¹ were performed to simulate three small scale feasibility experimental tests of explosions inside rigid chambers^{2, 3, 4}. Each of the tests is represented in a simplified form by an axisymmetric two-dimensional model with and without the presence of water. Each test includes a configuration wherein the water is placed close to the explosive such that the explosive may be considered to be immersed in the water. In addition, in one of the test series, the water was placed only on the sides of the explosive in order to determine the effect of water placement on the final gas pressure.

Three simplified models were analyzed using AUTODYN in its standard release form. Additional calculations were then made with AUTODYN, modified through use of a user subroutine, to account for heat transfer effects not represented in the standard version of the program.

2. Numerical Modeling

All of the analyses used the AUTODYN-2D general purpose, multi-material Euler processor to model the interior volume of the test chambers. All chamber walls were taken as rigid, and adiabatic, with a no flow condition (Euler default). Problems 1 and 2 consisted of charges detonated inside a sealed test chamber without any venting of the explosive products. In Problem 1, two joined Euler grids were used and in Problem 2 a single Euler grid was used to represent the chamber. The Problem 3 geometry consisted of a cylindrical chamber connected to a tunnel that was vented to the external atmosphere. Problem 3 was modeled using three joined Euler grids.

3. Material Modeling

All of the analyses were conducted using the Ideal Gas EOS (equation of state) to represent the air in the chamber, with an initial pressure of 101.33kPa (1 atmosphere). The water included in the analyses was modeled using the Two Phase expansion EOS with a Polynomial EOS used in compression. This standard model in AUTODYN gives a realistic description of both the single phase (liquid or vapor) and the two-phase (in which liquid and vapor co-exist) behavior of the water. Details of this model are given in the AUTODYN Theory Manual⁵. The explosive charges were modeled using standard Jones, Wilkins, and Lee (JWL) EOS data for TNT or C4, as included in the AUTODYN Material Library and further described in the AUTODYN Theory manual. The detonation energy of the explosive was modified for the Problem 1 analyses, as described later, to account for the heat of combustion.

4. Modified Analyses, with Energy Transfer

In addition to the use of the AUTODYN code in standard mode, additional analyses were performed that included a user subroutine that transferred energy between the gas materials (air/explosive products) and the water/vapor when the materials co-existed in mixed material Eulerian cells. A summary of the algorithm used in these modified analyses is given below:

- 1) Temperature was calculated for each material (air/products, water/vapor). The Two Phase EOS was modified to output temperature. If the water is on the saturation curve or in the two-phase region, the temperature is known. If the water is above the vapor side of the saturation curve, the temperature is calculated from ' $Pv = RT$ '. The calculated temperature is passed back to subroutine STATE (AUTODYN's primary equation of state solver). The air temperature was calculated using a constant C_v (specific heat), set to give a temperature of 288K at ambient conditions. The temperature in the explosive products was again calculated assuming a constant C_v . The value of C_v was taken as the average value over an expansion range of 10 to 100 times the explosive initial volume using data calculated in Cheetah⁶ version 1.40.
- 2) Each calculation was initially executed without any energy transfer until the explosive had expanded by a factor of approximately 10 from its initial volume. At this time the explosive EOS was changed to an ideal gas and the temperature in the detonation products was initialized by dividing the local internal energy by C_v .
- 3) For the remainder of each analysis, energy was transferred between any gas (detonation products/air) and two-phase water material in mixed material cells. The quantity of energy transferred was intended to reduce the temperature difference between the gas and the water/vapor in the cell at an arbitrary rate of 1% per microsecond. Other rates were not tested but could be the subject of further work. The internal energy in each material was updated based upon the energy transfer and the new values stored. The new temperature in the ideal gas material was calculated directly from the updated internal energy using the appropriate value of C_v . Typically, the energy transfer was from the gas to the water/vapor. However, if the two-phase material had a higher temperature than the gas, energy was transferred to the gas.

The above energy transfer procedure is somewhat ad hoc, but does address the general issue of heat transfer between the constituents. This relatively simple modification to the standard AUTODYN code yields quite reasonable results compared with the experimental tests and correlates well with the observed mitigation of gas pressure.

5. Problem 1 – NCEL Tests, Simplified Model

Two configurations were calculated and the results compared with experiment. The first has 4.67 lbs. of TNT and air in a cylindrical chamber of volume 1150 ft³, as shown in Figure 1-1. An axisymmetric model is used with a plane of symmetry allowing only half of the setup to be modeled. The explosive and room are modeled as cylinders of equal height and diameter.

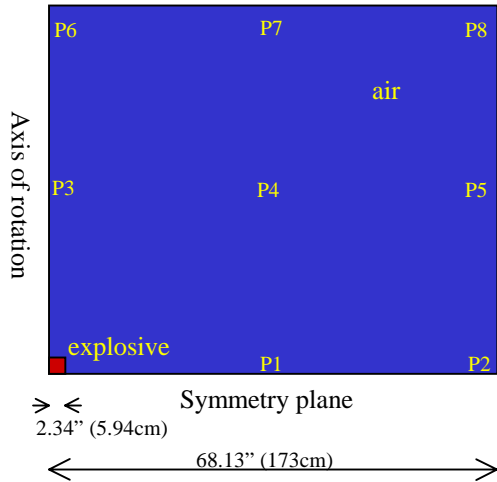


Figure 1-1. Explosive only

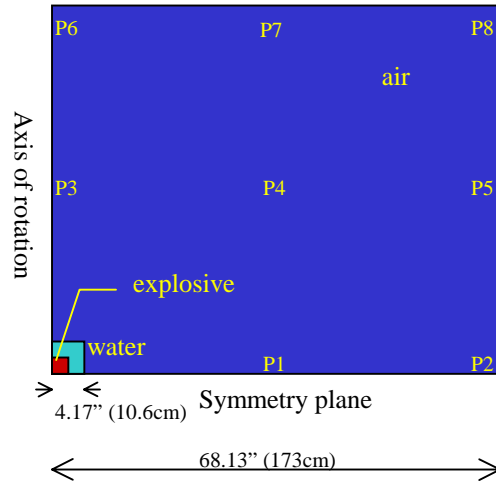


Figure 1-2. Explosive and water

The second configuration, as shown in Figure 1-2, is identical except for the inclusion of 13.5 lbs. of water also modeled as a cylinder of equal height and diameter surrounding the explosive.

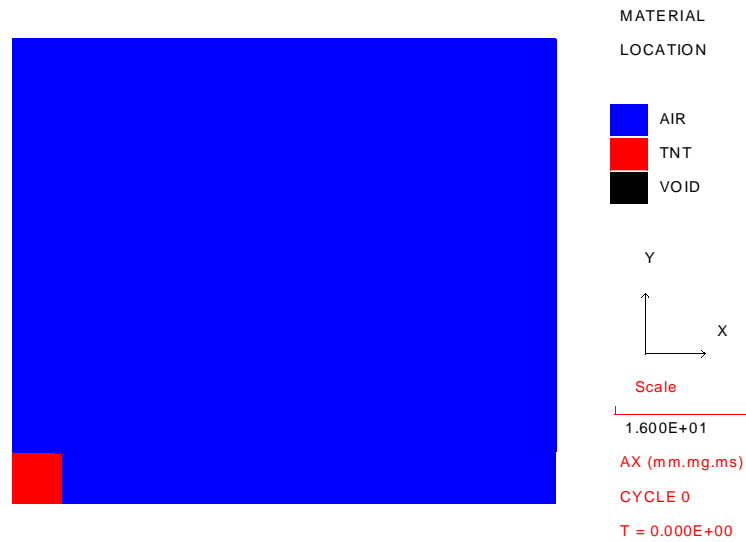


Figure 2. Initial material location for Problem 1 (Bare charge), runs 1 and 2
(Detailed model, 500x500 mm)

Figure 2 shows the material location plot, for the bare charge runs at time = 0.0. The numerical model covers a finely zoned 500mm square portion at the center of the chamber (lower left corner of the model). The mesh resolution is 100 x 5mm square cells in each direction (total of 10^4 cells). This detailed model was executed until just before the blast wave reached the edge of the mesh at a time ~ 0.12 msec as shown in Figure 3.

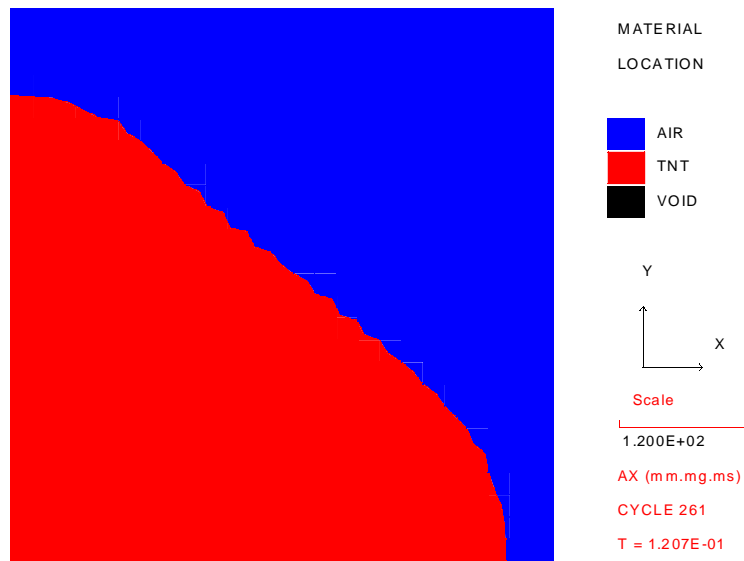


Figure 3. Initial explosive expansion in fine mesh

The mesh was then dezoned by a factor of 4 in each direction. Dezoning is a standard feature of AUTODYN that combines finer Eulerian cells into coarser cells, thereby reducing the overall number of cells in the mesh. Dezoning by a factor of 4, results in a new mesh with cells 20 mm square, and a mesh size of 25 x 25.

At this same time, the JWL equation of state of the TNT is changed to an ideal gas EOS with $\gamma = \omega + 1$ (1.35) and with a reference density a factor of 1000 lower than the JWL reference density. This transformation is justified since the JWL equation of state, at large expansions, asymptotes to an ideal gas. The transformation to an ideal gas with a low reference density yields a more numerically accurate calculation for the subsequent explosive product behavior. Further discussion of this technique is provided in the AUTODYN Remap Tutorial ⁷.

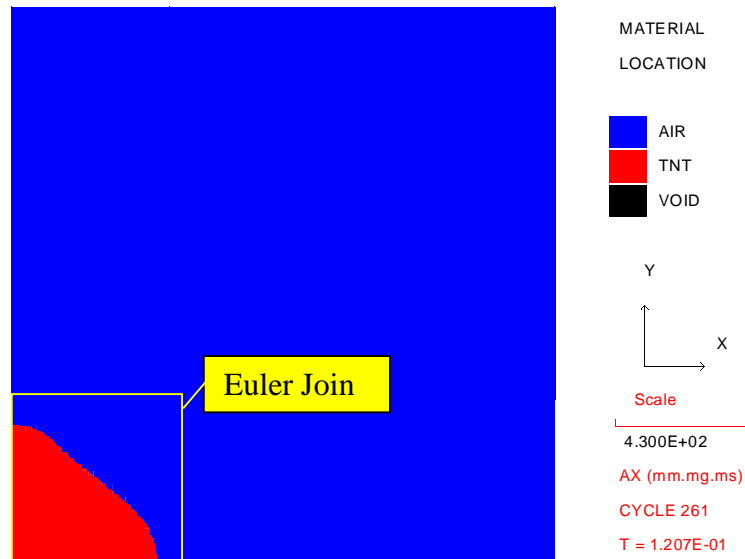


Figure 4. Material locations after dezone and joining of second mesh

A second Euler grid was then added, with 20mm square cells, to extend the model to encompass the remainder of the interior volume of the test chamber. The material locations of the resulting larger mesh is depicted Figure 4. The two Euler grids were joined along their common edges. Eight gauge (target) points were defined in the outer subgrid corresponding with the locations indicated in Figure 1. A user subroutine was used to convert overpressures to psi (from the metric units of the calculation) at each gauge point as well as an average overpressure for all eight gauge points.

TNT is 74% oxygen deficient. The air in the chamber contains 5.9 times the mass of oxygen required to compensate for the oxygen deficiency in the charge. For this reason, and because of better agreement with experiment (see Runs 1 and 2 below), these models used an increased TNT detonation energy based on the ratio of the TNT heat of combustion to its heat of detonation, as determined from the US Department of the Army Technical Manual TM5-1300⁸, Table 2-1. This scaling gave good agreement with the experimental gas pressure for the bare charge case.

Four runs were completed for Problem 1. Each analysis was executed for 30ms. Table 1 summarizes the results.

Run	Description	Average Gas Pressure (1-8) psig	
		Experiment	Calculated
1	Bare charge with standard TNT data	51.3	19.0
2	Bare Charge with scaled energy for heat of combustion	51.3	48.3
3	Immersed charge, scaled energy, no energy transfer	5.8	30.3
4	Immersed charge, scaled energy, with energy transfer	5.8	24.3

Table 1. Problem 1, Comparison of experiment and calculation

The experimental values are taken from Reference 2 (Keenan et al) that describes the NCEL tests. The 'Calculated' values are the average residual gauge pressure in AUTODYN at the eight gauge locations as measured from 25 to 30ms.

The bare charge gas pressure, with scaled energy to account for heat of combustion, is within ~6% of the experimental value. The immersed charge analysis results are not as close, but the energy transfer calculation does show the trend of further reducing the gas pressure. It is surmised that, in the experiment, the water cools the explosive products sufficiently to inhibit complete combustion of the products. Figures 5 to 8 show the distribution of material for each case after 30 msec.

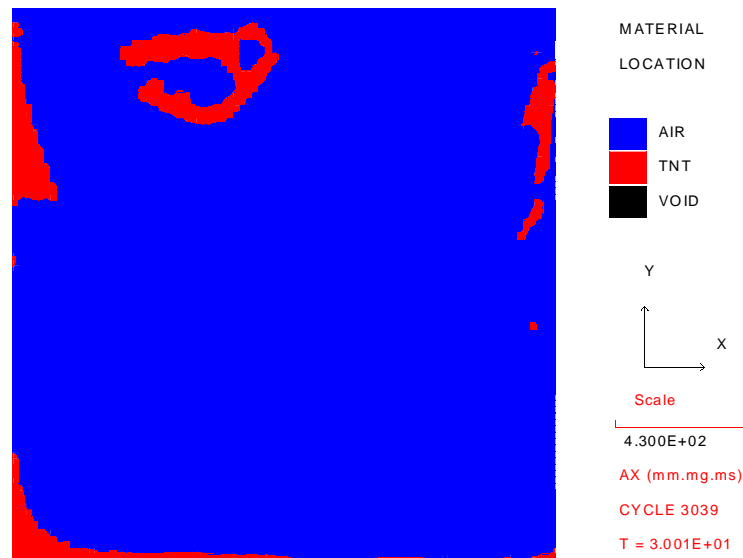


Figure 5. Run #1, Bare charge, standard TNT at 30 msecs

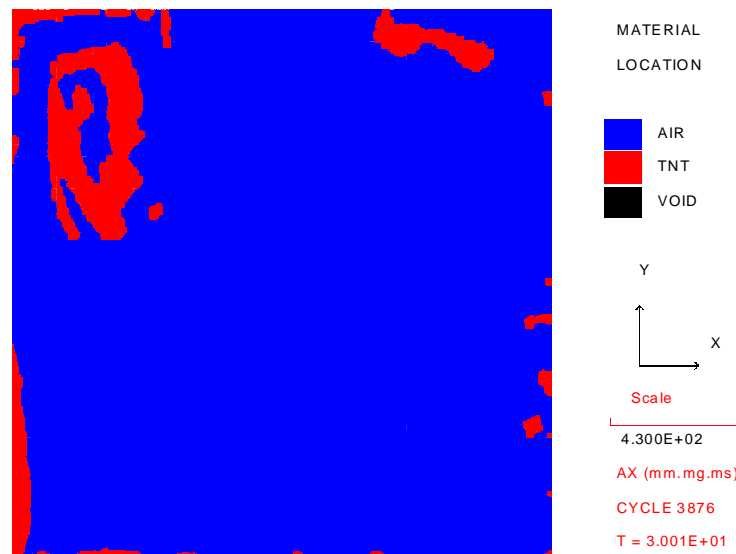


Figure 6. Run #2, Bare charge, scaled TNT, at 30 msecs

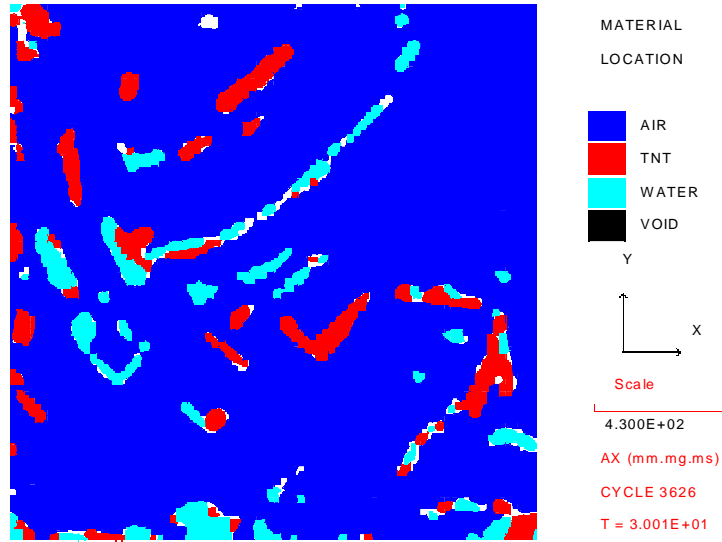


Figure 7. Run #3, Immersed charge, scaled energy, no energy transfer, at 30 msecs

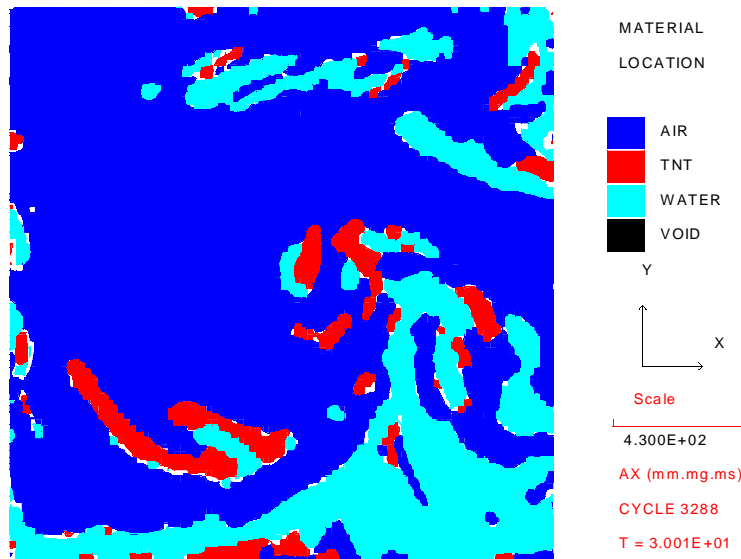


Figure 8. Run #4, Immersed charge, scaled energy, with energy transfer, at 30 msecs

The material locations at the end of the analysis show marked differences for the Run 3 (Figure 7) and Run 4 (Figure 8) analyses, without and with energy transfer. The water/vapor volume is clearly shown to be much greater with energy transfer (Run 4). Figure 9 shows the pressure histories at the center of the tank and the comparison with the experimental residual pressure.

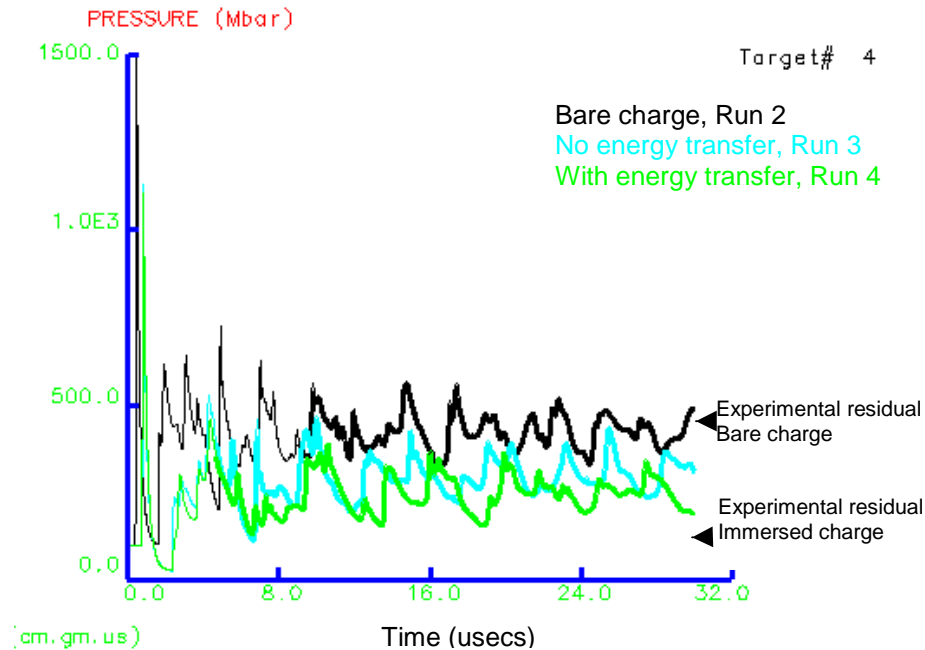


Figure 9. Pressure histories at Gauge 4 (Center of Tank)
Comparison with experimental residual pressure

6. Problem 2 – Huntsville Tests, Simplified Model

Three configurations were calculated for the tests described in Reference 3 (Marchand, et al). The first one, the control setup, is for a bare explosive charge and air in a cylindrical chamber as shown in Figure 10. An axisymmetric model is again taken and only half of the setup is modeled. The explosive is modeled as a cylinder of equal height and diameter. The second configuration, an immersed explosive, includes 20 lb. of water also modeled as a cylinder of equal height and diameter surrounding the explosive. Numerical results from these two configurations are compared with the experimental results. A third configuration, a surrounding water cylinder, was analyzed in which the water is placed only around the explosive on the sides, such that the explosive is not fully immersed, but the same amount of water as the second configuration is used. No experimental data was available for this last configuration.

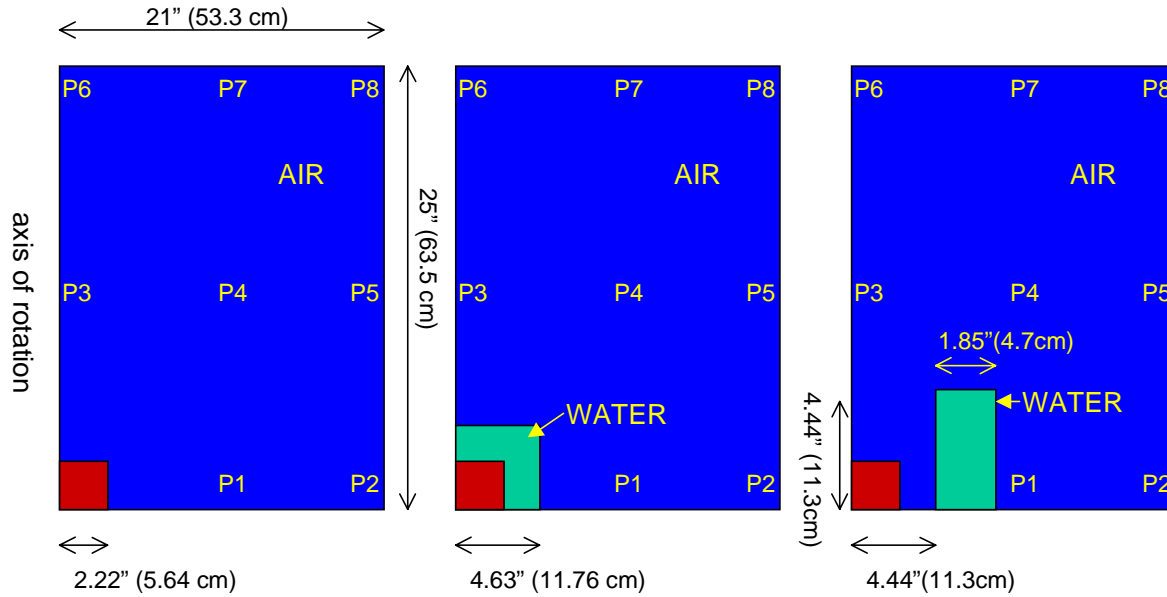


Figure 10. Control setup

Immersed explosive

Water cylinder

The Marchand paper describing the Huntsville tests refers to a 3.13lb C4 charge with a TNT equivalency of 4lb. This implies that 1kg of C4 is equivalent to 1.28kg of TNT. This equivalency would appear to be the average of the peak pressure and impulse equivalency quoted in CONWEP^{9, 10} for external air blast. There is however no guarantee that this value of TNT equivalency has any relevance to the long term gas pressure that a charge will produce in a sealed chamber. In order to follow the actual experimental setup more closely, C4 was used in all of the analyses and not a 4 lb “equivalent” TNT charge. This choice is also further validated by the reasonable agreement achieved in the control setup (bare charge) case between calculated and experimental results when using the “real” 3.13lb C4 charge.

C4 is 91% RDX and RDX is 21% oxygen deficient. There is a factor of 1.05 times the additional oxygen required to balance the explosive products contained in the chamber. However, this case gave best agreement with the bare charge experiment results using standard JWL data without scaling for the heat of combustion.

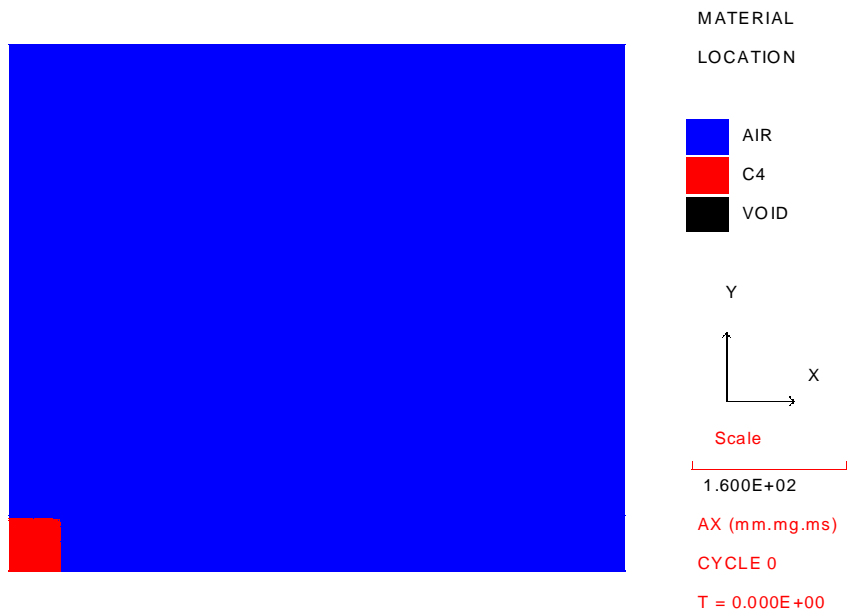


Figure 11. Calculational setup for Huntsville Run 1 (Bare Charge)

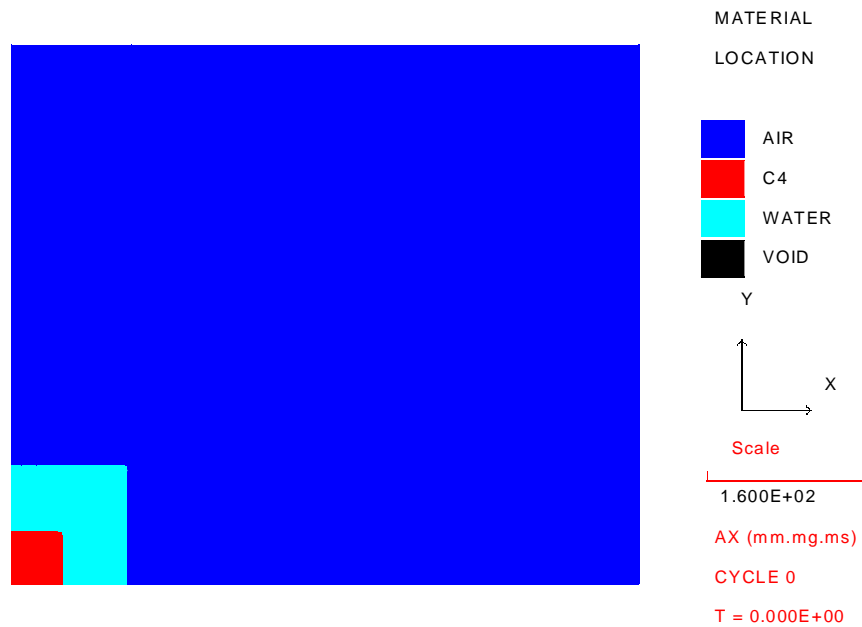


Figure 12. Huntsville Runs 2 and 4, Explosive immersed in water

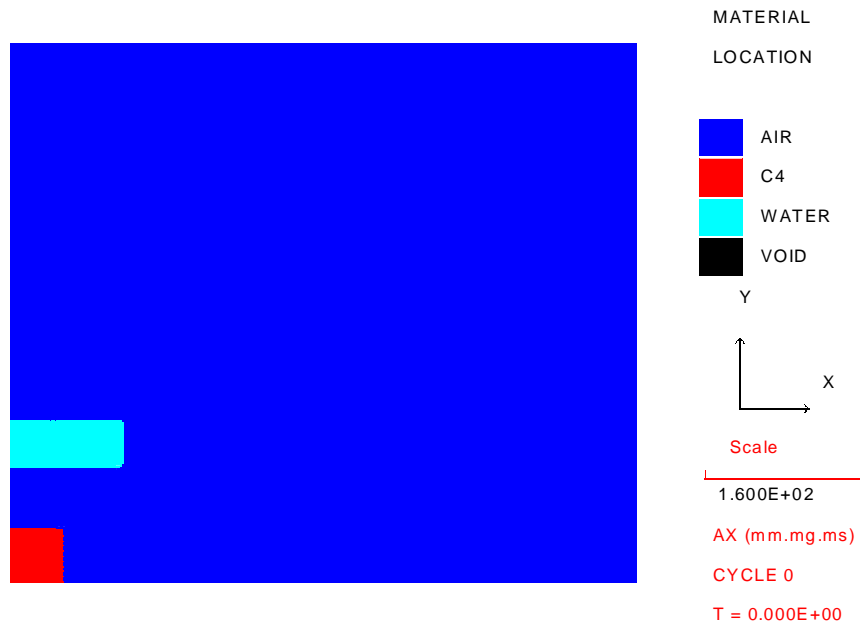


Figure 13. Runs 3 and 5, Water cylinder around explosive

Each model was set up using a single Euler subgrid with approximately 5mm square cells. The initial material locations are as depicted in Figures 11-13. (Note that the x-axis is the axis of symmetry in AUTODYN, and thus the AUTODYN models are “rotated” from the configurations shown in Figure 10.)

The models were run until the explosive products had expanded by a factor of about 10 from the initial explosive density. The mesh was then dezoned by a factor of 2 in each direction, and the JWL EOS changed to an ideal gas EOS with $\gamma=\omega+1$ and reference density a factor of 1000 lower than the JWL reference density.

Eight gauge points were defined in the chamber as specified in Figure 10. A user subroutine was used to calculate over pressures in psi at each gauge point, as well as an average over-pressure for all eight gauge points.

Five different analyses were completed for Problem 2 as shown in Table 2. Each analysis was executed for 5ms.

Run	Description	Average Gas Pressure (P1-8) psig	
		Experiment	Calculated
1	Bare charge, standard C4 JWL data	350	425
2	Immersed charge without energy transfer	100	174
3	Charge plus water cylinder	N/A	356
4	Immersed charge with energy transfer	100	95.1
5	Charge plus water cylinder with energy transfer	N/A	218.4

Table 2. Problem 2 (Huntsville) Analyses, Comparison of Experiment and Calculation

These results show reasonable agreement for the bare charge case, with ~20% overprediction. Increasing the C4 detonation energy, to account for heat of combustion, would lead to even higher calculated gas pressures and less agreement with the experimental result. Immersing the charge in water gives a significant decrease in the calculated gas pressure (~60%), though not quite as much as the reduction seen in the experiments (~71%). Including energy transfer between the materials gives a further significant decrease in the calculated gas pressures. The calculated gas pressure for Run 4, which is the immersed charge with energy transfer, is within 5% of the experiment. Experimental results are not available for Runs 3 and 5 with a water cylinder placed close to the charge. Note that the water cylinder (Run 3) provides a ~16% reduction in gas pressure while in Run 5 where the energy transfer mechanism is invoked provides a ~49% reduction. As shown in Table 3 below, the water cylinder is shown to be not as effective as the complete immersion case, but indicates that substantial reductions are still available for situations wherein it is not possible to deploy water around the explosive to achieve complete immersion.

Run	Description	Average Gas Pressure (P1-8) % Reduction	
		Experiment	Calculated
1	Bare charge, standard C4 JWL data	-	-
2	Immersed charge without energy transfer	72%	59%
3	Charge plus water cylinder	N/A	16%
4	Immersed charge with energy transfer	72%	78%
5	Charge plus water cylinder with energy transfer	N/A	49%

Table 3. Comparison of Percentage Reduction in Gas Pressure from Bare Charge Experiment vs. Calculation

Figure 14. below depicts the placement of the air and explosive at 5 msecs for the bare charge.

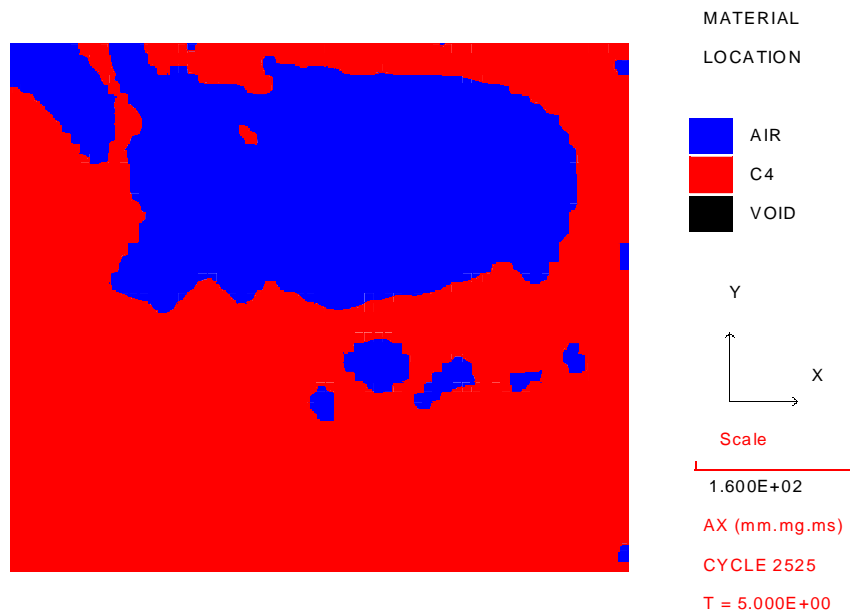


Figure 14. Run 1 (Bare Charge) at 5 msecs

The energy transfer calculations in Runs 4 and 5 again had the effect of significantly increasing the proportion of the chamber volume occupied by two phase material (water/vapor). This is shown clearly at the end of the analyses in Figures 15-18 below:

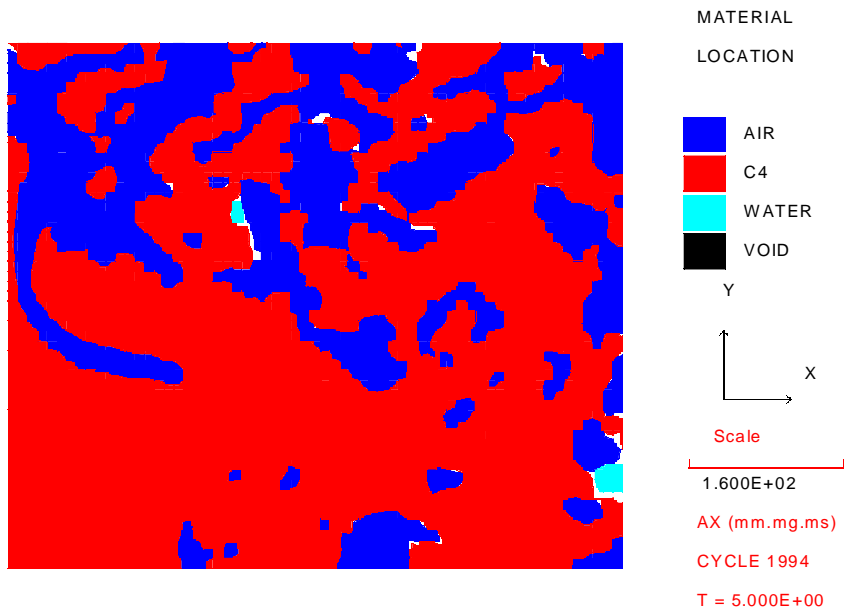


Figure 15. Run 2 (Immersed Explosive, No Energy Transfer)

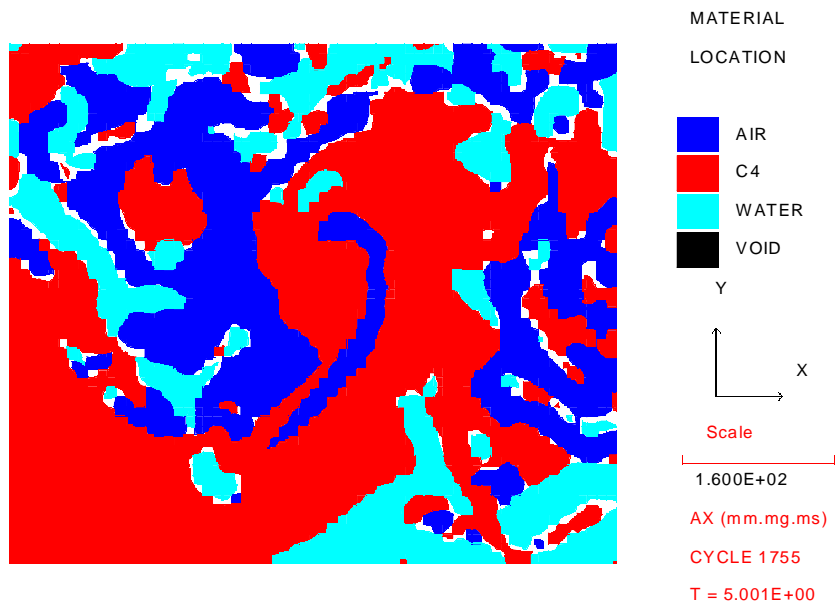


Figure 16. Run 4, Immersed charge with energy transfer
(Note: Increased water/vapor volume)

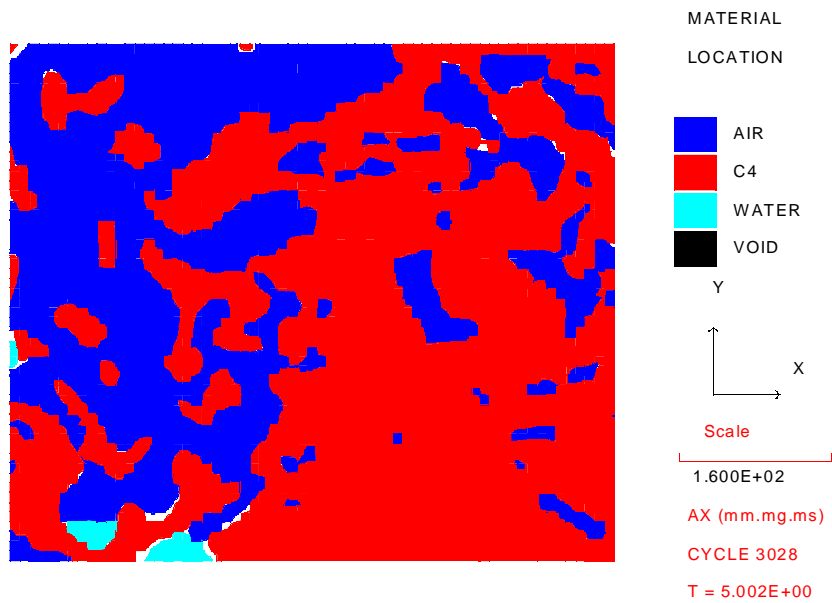


Figure 17. Run 3, Water cylinder surround, no energy transfer

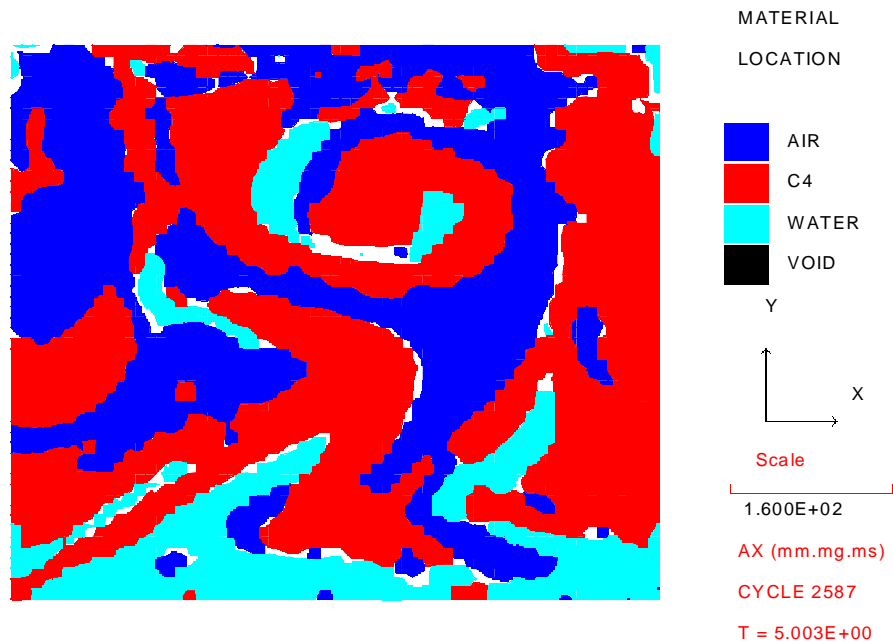


Figure 18. Run 5, (Water Cylinder Surround, with Energy Transfer)
(Note: Increased Water/Vapor Volume)

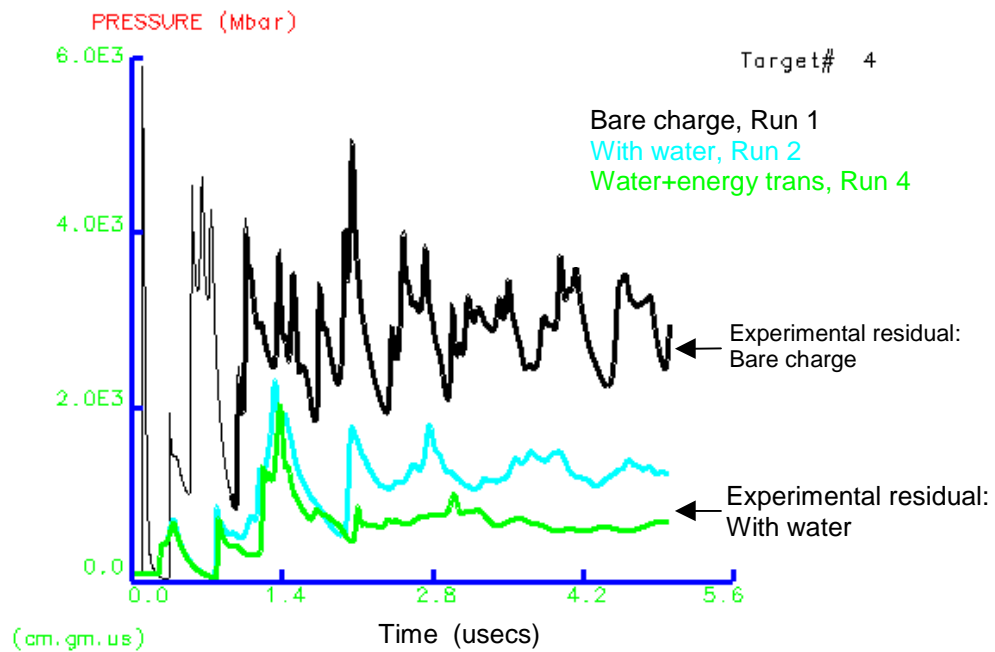


Figure 19. Pressure Histories at Gauge 4 (center of tank) for bare and immersed charge
Comparison with experimental residual

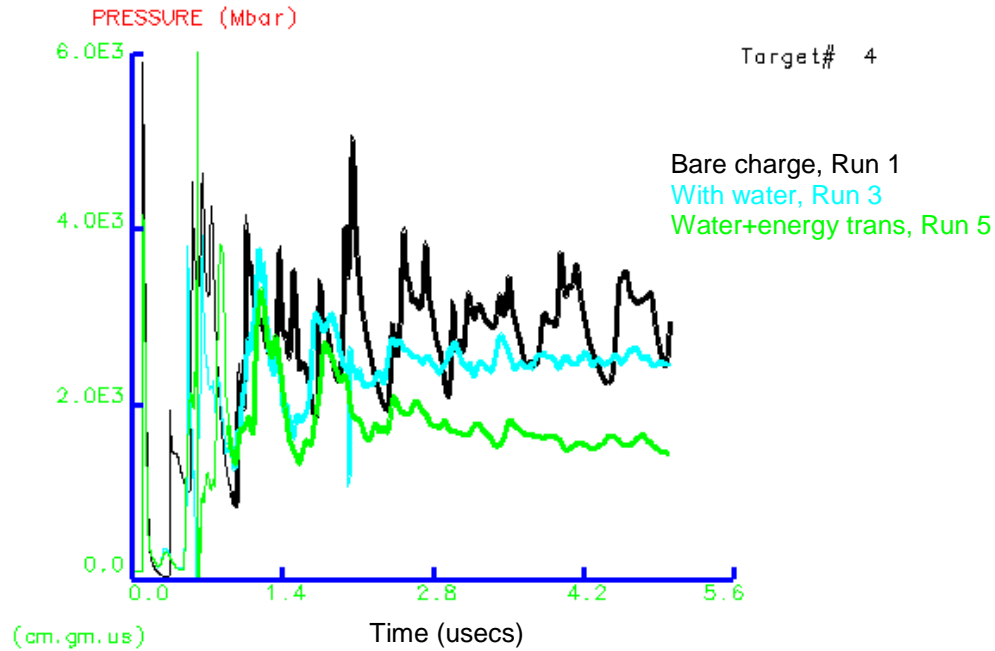


Figure 20. Pressure Histories at Gauge 4(center of tank) for bare and water cylinder
Note effect of energy transfer.

Figure 19. shows the pressure history in the center of the tank. The mitigating effect of the water is pronounced and correlation with the experimental residual pressure is excellent. Figure 20, for the water cylinder surround, also shows the decrease in pressure. No experimental data was available to compare against.

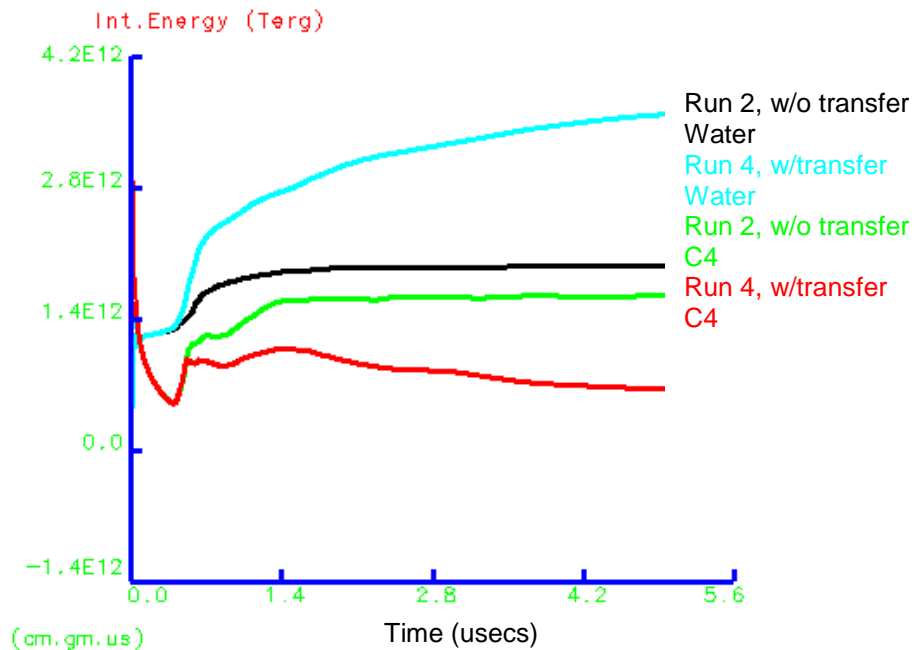


Figure 21. Global internal energy partition between C4 and Water/Vapor
Run 2(no energy transfer) and Run 4 (with energy transfer)

Figure 21 illustrates the internal energy partition histories for the C4 and water/vapor with (Run 4) and without (Run 2) the energy transfer mechanism. An equilibrium is reached in both cases but with substantially more energy transferred from the C4 to the water/vapor when the energy transfer mechanism is invoked.

7. Problem 3, Swedish Tests, Simplified Model

For Problem 3, from Reference 4 (Forsén et al), two configurations were calculated. The first has 200 g of C4 explosive and air in a cylindrical chamber of volume 0.061 m^3 , as shown in Figure 22. An axisymmetric model is used. The C4 is assumed to have a density of 1.66 g/cc , and is modeled as a cylinder of equal height and diameter (radius = 2.68 cm ($1.05''$)).

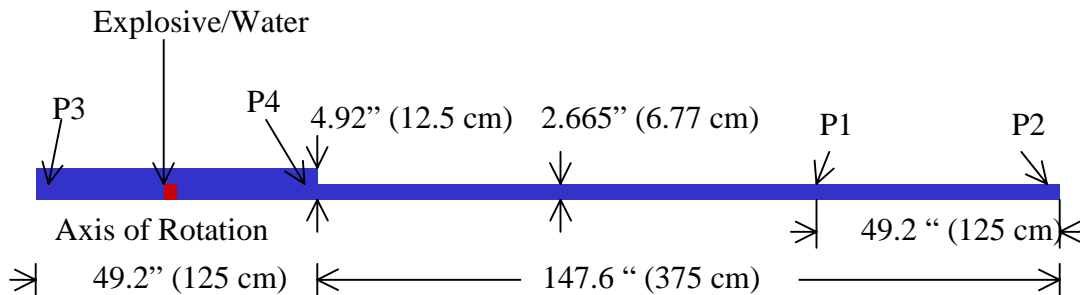


Figure 22. Model of the KLOTZ Club Tunnel in Alvaden, Sweden

The second configuration includes 600 g of water also modeled as a cylinder of equal height and diameter surrounding the explosive (radius = 4.86 cm ($1.91''$)). Numerical results are compared with experimental values from Reference 4.

These analyses used three Euler grids to model the chamber, the tunnel and a small region outside the tunnel mouth. The chamber was initially set up with approximately 2.5mm square cells and executed until the explosive products had expanded by a factor of about 10 from the initial explosive density. The initial material locations for Run 1 (bare charge) are shown in Figure 23.

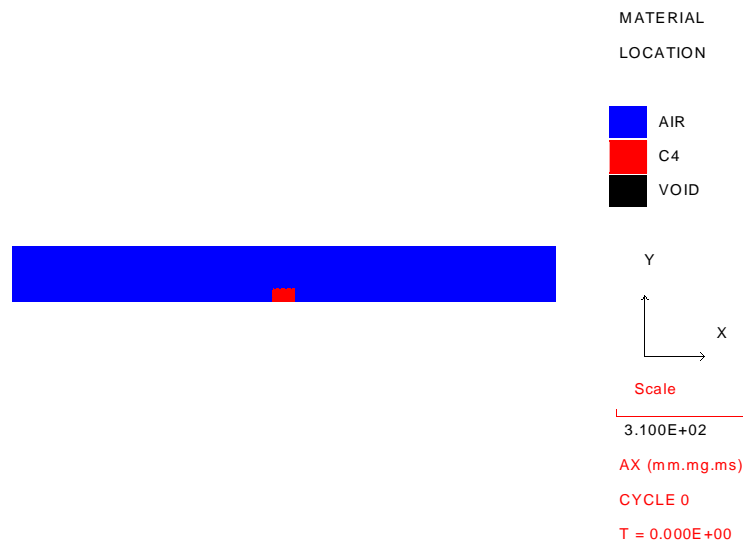


Figure 23. Run 1, Bare charge, initial setup, chamber only

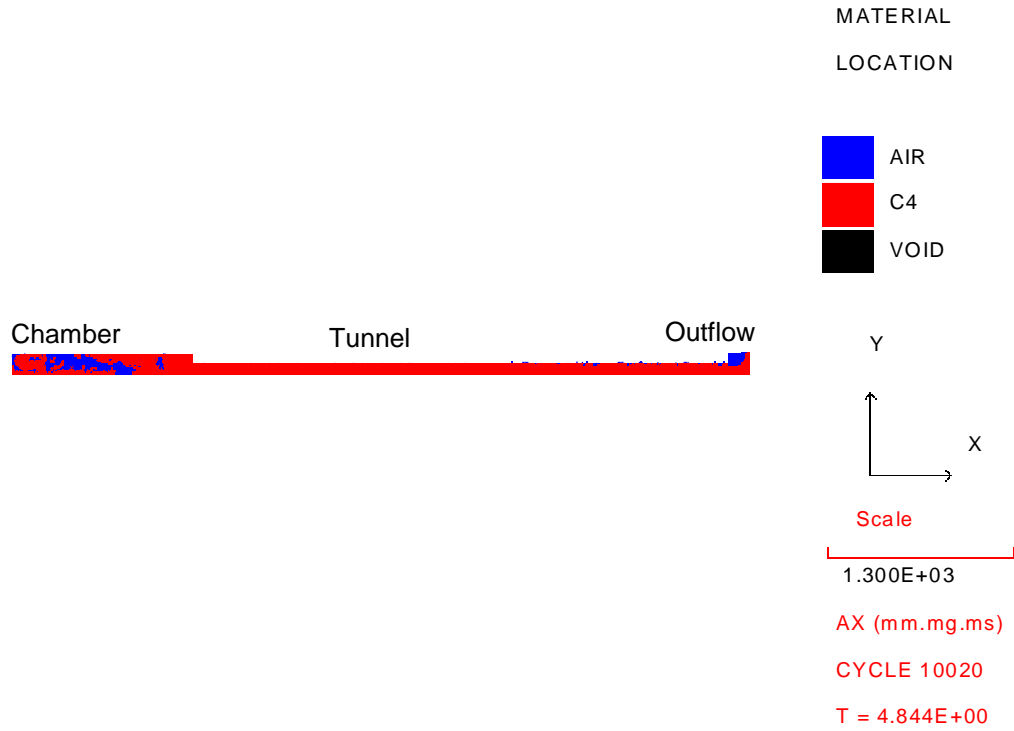


Figure 24. Run 1, Bare Charge at 4.8 msecs, Tunnel and Outflow joined to Chamber

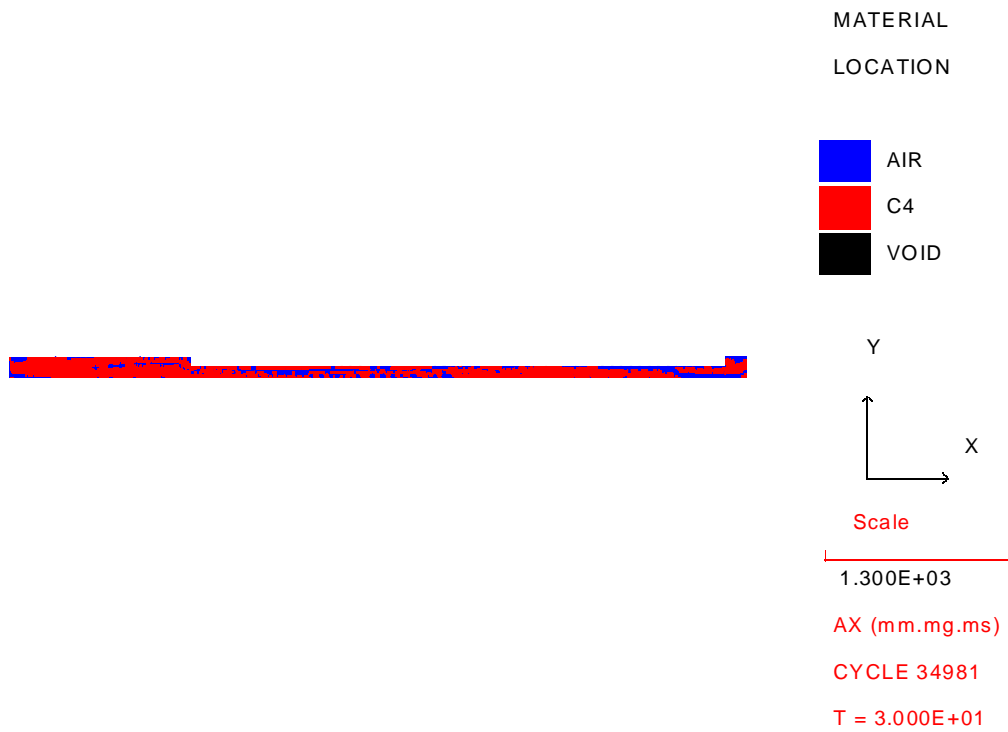


Figure 25. Run 1, Bare Charge at 30 msecs

At a time of 0.075 msecs, the mesh describing the chamber was dezoned by a factor of 2 in each direction. A tunnel subgrid and exterior subgrid were joined to the original chamber as shown in Figure 24. As in Problems 1 and 2, for reasons of accuracy, the JWL EOS was changed to an ideal gas EOS with $\gamma=\omega+1$ and reference density a factor of 1000 lower than the JWL reference density. An outflow boundary condition was used to allow material to vent from the exterior subgrid outside the tunnel mouth. All three subgrids were dezoned by a factor of 2 in both directions at about 5ms, and the problem calculated out to 30 msecs as shown in Figure 25. Four gauge points were defined, two in the chamber and two in the tunnel, as per Figure 22. A user subroutine was used to calculate overpressures in psi at each gauge point.

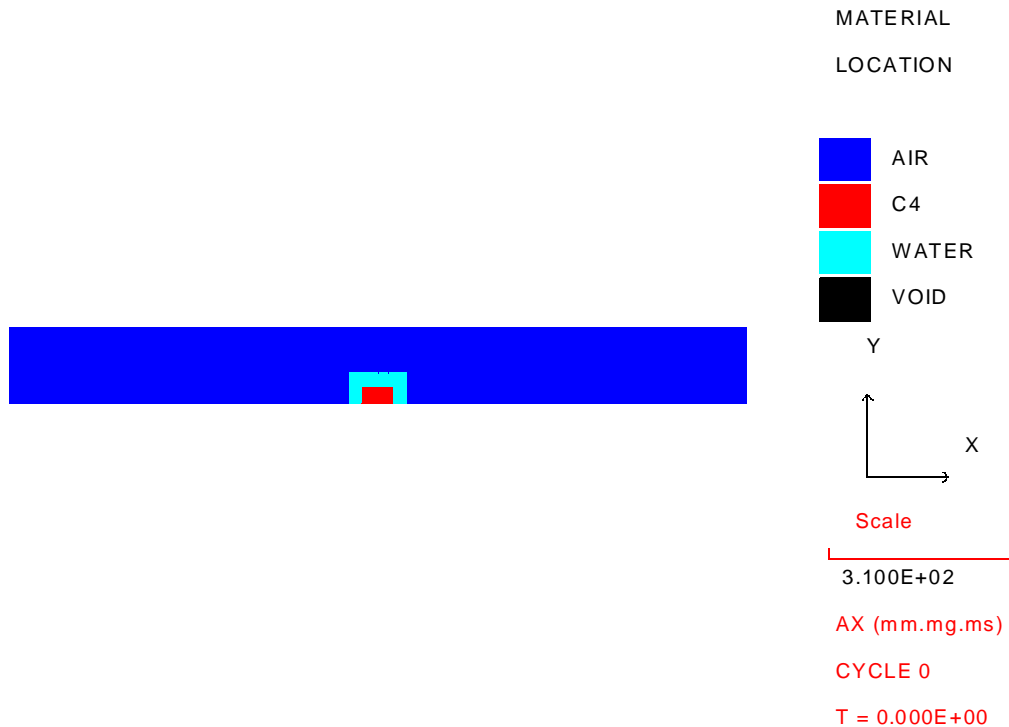


Figure 26. Initial Configuration, Runs 2 and 3, Immersed Charge

Figure 26. shows the material locations for the immersed charge Runs 2 and 3. As in the bare charge (Run 1), the initial expansion is carried out in a fine mesh with only the chamber modeled. Then, the chamber is dezoned and the tunnel and outflow added. The problems were then calculated out to a time of 40 msecs as shown in Figures 27 and 28. Significantly, Run 3, which includes energy transfer between the C4 products and the water/vapor shows substantially more volume occupied by the water/vapor material. This increased volume of water/vapor correlates to the lower peak pressures and lower impulses.

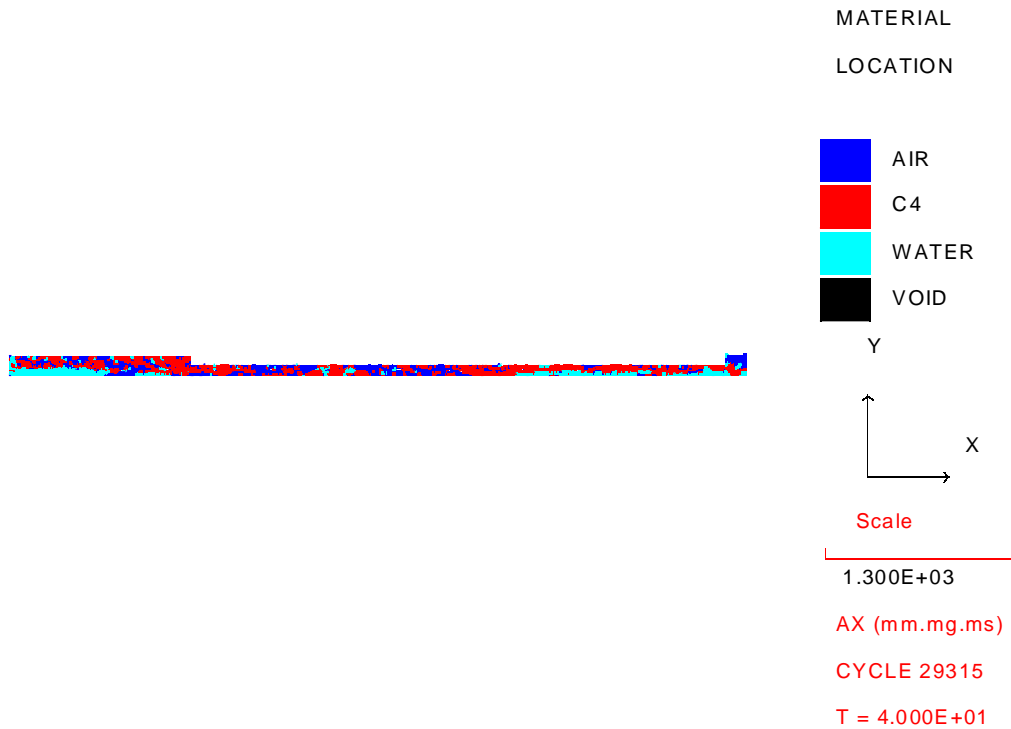


Figure 27. Run 2, Immersed Charge, No Energy Transfer, at 40 msec

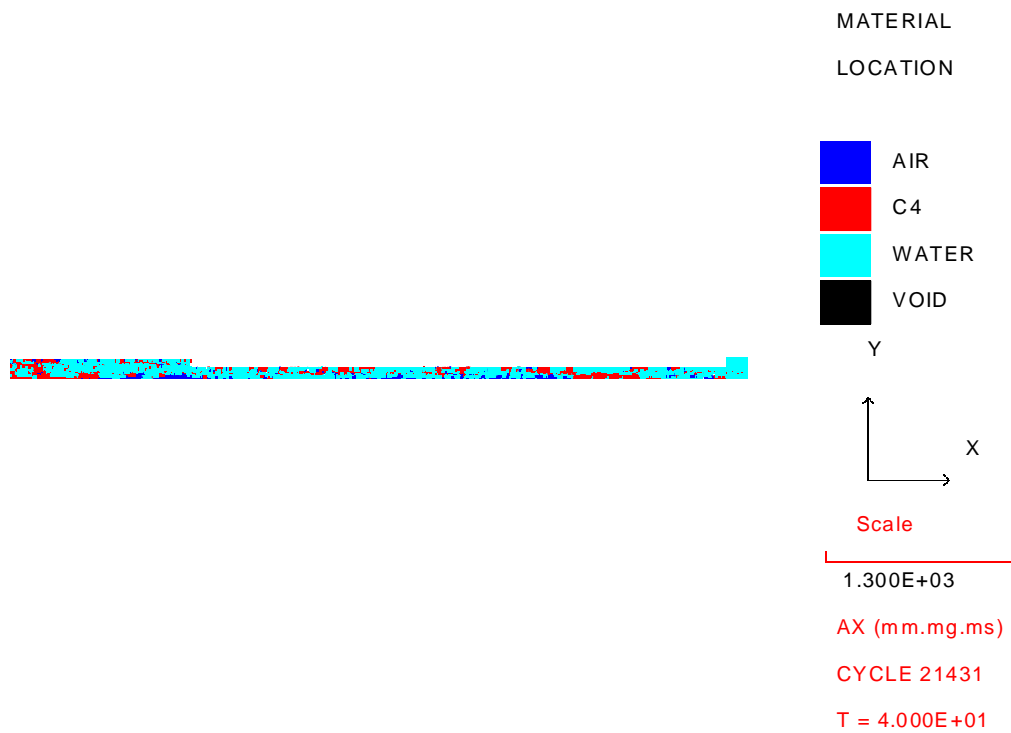


Figure 28. Run 3, Immersed Charge with Energy Transfer
Note: majority of volume is water/vapor

All of these models used standard C4 data. There is a factor of 0.4 times the additional oxygen required to balance the explosive products contained in the chamber. As with Problem 2, good agreement with experimental results for the bare charge case was obtained using standard JWL data for C4.

The results given in Table 4 below are peak pressures and impulses at gauge point 2 located at the end of the vent tunnel. For the bare charge, the calculation shows a higher peak pressure, but the impulse is almost exactly that observed in the experiment. For the immersed charge runs, it should be noted that the experimental results are for 400g of water while the numerical results are for 600g of water and cannot be compared directly. Nevertheless, the mitigation of pressure and impulse due to the presence of water is clearly demonstrated.

Run	Description	Gauge #2 Peak Pressure (kPa)		Gauge #2 Impulse (kPa-ms)	
		Experiment	Calculation	Experiment	Calculation
1	Bare charge	2500	3970	11500	11400
2	Immersed charge without energy transfer	1670	2600	7920	10500
3	Immersed charge with energy transfer	1670	2270	7920	8400

Table 4. Problem 3, Comparison of experiment and calculations

In Reference 4, there were also some experiments carried out with 600g of water and the results of these are presented in Figures 3 and 4 of the Reference as ratios of the peak pressure or impulse for the water encased charges compared with the bare charge case. Using this experimental data, we can better compare the calculational results that were similarly performed with 600 g of water. As shown in Table 5 below, at Gauge P2, experimental results give a peak pressure reduction of 45-55%. This compares with a calculated reduction of 43% for Run 3 with energy transfer. For impulse, the experiments give a range of 18 to 28% reduction at P2 compared with a calculated reduction of 26% for Run 3 with energy transfer.

Peak pressure reduction (600 g water)		Impulse reduction (600 g water)	
Experiment	Calculation	Experiment	Calculation
45-55%	43%	18-28%	26%

Table 5. Reductions due to water suppression, experiment vs. calculation

Thus, the AUTODYN calculations, including energy transfer, provide excellent correlation with the pressure and impulse reduction effects seen in the experiments.

8. Conclusions and Further Work

The efficacy of the use of water to mitigate the gas pressure and impulse from an explosive was borne out by the calculations performed with AUTODYN-2D. In each of the three problems wherein no water was present, AUTODYN compared favorably with the experimental results. In Problem 1, a very oxygen deficient explosive (TNT) in an oxygen rich situation, it was found necessary to scale the explosive energy to include the heat of combustion. In Problems 2 and 3, which were performed with an explosive (C4) less deficient in oxygen than TNT and an environment that was not oxygen rich, no scaling of explosive energy was required.

When water was introduced, the calculations with AUTODYN in standard mode demonstrated reductions in gas pressure and impulse but not to the extent observed in experiment. An energy transfer mechanism between the explosive products/air and water/vapor was then added to the standard AUTODYN code through use of a user subroutine. With the energy transfer invoked, the AUTODYN analyses demonstrated substantial reductions in the gas pressures and impulses correlating very well with experimental measurements.

However, one should be cautioned that the calculational and modeling techniques employed in these simple problems may not guarantee similar results for more complex problems. It is suggested that AUTODYN, as modified, be further validated against additional and more complex cases of varying geometry, different explosives, and different material ratios.

In addition, it should be noted that the energy transfer mechanism, undoubtedly should be further enhanced and validated. The energy transfer did produce very reasonable results for these problems. The creation of water/vapor volume due to energy transfer from the detonation products is consistent with the postulated mitigating physical mechanisms. However, the rate of energy transfer used in the calculations was admittedly somewhat ad hoc. Suggested future work could be to base the actual rate upon additional physics associated with the heat transfer between the materials in the problem. This further work would presumably lead to better results for situations such as Problem 1, wherein the explosive/air/water ratios appeared to inhibit the complete combustion of the detonation products as compared to the bare charge.

Nevertheless, based upon these validating calculations, the AUTODYN code, with the added user subroutine, provides a very useable tool for studying the deployment of water around explosives for mitigation purposes. Other geometries can easily be explored as well as different explosive/air/water ratios.

9. References

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